FORMATION AND DYNAMICS OF BOOJUMS IN THE THIN LAYERS OF NEMATICS WITH HYBRID BOUNDARY CONDITIONS

Hiroyasu Toyoki
Department of Physics, Faculty of Education and Liberal Arts, Yamanashi University, Kofu 400, Japan

Phase Ordering of a nematic layer with hybrid boundary conditions is numerically studied. The upper boundary of the layer is homeotropic, where the director is forced to be perpendicular to the upper plane, and the director is forced to tangential to the plane at the lower boundary.

When a system is rapidly quenched from a disordered phase to an ordered phase, the spatial pattern of the order-parameter field coarsens through the annihilation of topological defects. For example, in three-dimensional nematic systems, disclination lines dominate the spatial patterns.

Defects in the hybrid nematic layer has been described by Lavrentovich and Nastishin (see references in [1]). Those are called *boojums*, whose core is bounded on the surface. After three-dimensional disclination lines annihilate, boojums take a crucial role in the dynamics. The main purpose of the present work is to investigate the formation and the pair annihilation process of boojums in the phase ordering.

A numerically efficient model for the phase ordering is the *cell-dynamical-system* (CDS). The phenomenological energy with the nematic symmetry (RP^2) can be written in the form $F = -\sum_{<\boldsymbol{r}\,\boldsymbol{r}'>} |\boldsymbol{\psi}(\boldsymbol{r}) \cdot \boldsymbol{\psi}(\boldsymbol{r}')|^2$ where $\boldsymbol{\psi}$ is a vector order-parameter. Assuming the simple relaxational dynamics (model A), we have

$$\begin{aligned}\boldsymbol{\psi}(\boldsymbol{r},t+1) &= \tau c \sum_{\boldsymbol{r}'} z_{\boldsymbol{r}\boldsymbol{r}'} \Big[(\boldsymbol{\psi}(\boldsymbol{r},t)\cdot\boldsymbol{\psi}(\boldsymbol{r}',t))\,\boldsymbol{\psi}(\boldsymbol{r}',t) - \frac{1}{2}\left(|\boldsymbol{\psi}(\boldsymbol{r},t)|^2 + |\boldsymbol{\psi}(\boldsymbol{r}',t)|^2\right) \\ &\quad \times \boldsymbol{\psi}(\boldsymbol{r},t)\Big] + (1+\tau)\boldsymbol{\psi}(\boldsymbol{r},t) - \tau|\boldsymbol{\psi}(\boldsymbol{r},t)|^2\boldsymbol{\psi}(\boldsymbol{r},t) \quad , \end{aligned} \tag{1}$$

where the sum is taken over the nearest-neighbor (NN) and the next-nearest-neighbor (NNN) cells.[2] We used parameters $\tau = 0.05$, $c = 0.1$, and $z_{\boldsymbol{r}\boldsymbol{r}'} = 1.0$ for NN and $z_{\boldsymbol{r}\boldsymbol{r}'} = 0.5$ for NNN. The initial configuration is given by a random number sequence $[-0.05, 0.05]$ for each component of $\boldsymbol{\psi}$, and the periodic boundary condition is assumed.

Figure 1 shows some snapshots in the annihilation process of disclination lines. The lines terminate at the lower boundary or form a closed ring. The former case is interpreted as the upper half part of a ring if the mirror image is assumed below the boundary. Disclination rings can be classified into two groups by whether a ring become a singular point (hedgehog) or nothing when collapsing. In the present system, disclinations terminating at the boundary shrink and become a boojum or annihilate. Thus, the system exhibits a crossover from the 3d growth (disclination lines) to the 2d growth (boojums). Figure 2 shows Schlieren patterns in the annihilation process of boojums.

According to the experimental work due to Lavrentovich and Rozhkov[1], the elastic energy (the deformation of director) is localized in a stringlike region between a pair of boojums. As a result of this structure, the distance of a pair linearly decreases as time. However, in the present simulation, such a string has not been observed. The behavior of the boojums is similar to vortices in the 2d XY spin model. Figure 3 shows the time evolution of the separation between the boojums. The separation decreases as $(t_0-t)^{1/2}$. This indicates that the interaction between boojums is logarithmic.

We examined the effect of the surface term of energy as a possibility for the mechanism of the formation of strings between boojums. The director pattern would be affected by the K24 term whose energy density is written as $f_s = -K_{24}\nabla\cdot[\psi(\nabla\cdot\psi)+\psi\times\nabla\times\psi]$. However no evidence have been found for the string-like deformation.

[1] O. D. Lavrentovich and S. S. Rozhkov, Sov. Phys. JETP Lett. **47**, 255 (1988).

[2] H. Toyoki, J. Phys. Soc. Jpn. **63**, 4446 (1994).

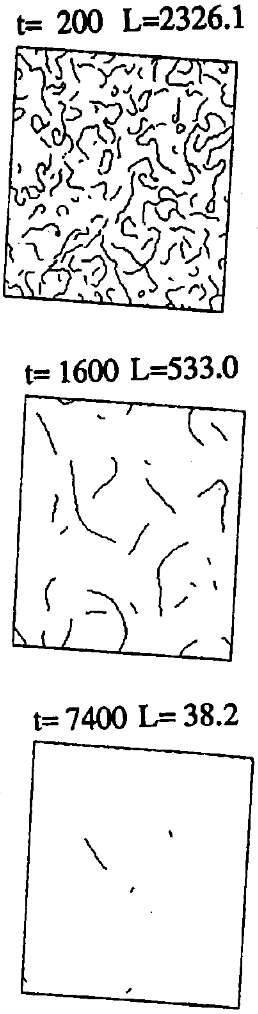

Fig.1 Bird's-eye snapshots of a growth process of disclination lines in a $128^2\times 4$ system. (*left*)

Fig.2 Schlieren patterns in the same run as Fig.1.

Fig.3 Separation d between a pair of boojums vs. time until the annihilation time t_0. The solid line indicates the slope 0.43. (*right*)